AD-A258 182

IMENTATION PAGE

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1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
		FINAL REPORT 01 SEP 88 to 31 JUL 92

4. TITLE AND SUBTITLE	5. FUNDING NUMBERS
METHODS AND CONVERGENCE ANALYSIS IN LARGE SCALE NONLLINEAR OPTIMIZATION	AFOSR-88-0267 61102F 2304/A8 (2)
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9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NM Bolling AFB DC 20332-6448	10. SPONSORING/MONITORING AGENCY REPORT NUMBER AFOSR-TR- 92 0979
11. SUPPLEMENTARY NOTES	
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited.	12b. DISTRIBUTION CODE

DTIC ELECTE DEC 0 4 1992 S A D

13. ABSTRACT (Maximum 200 words)

A new algorithm for the solution of large-scale nonlinear constrained optimization problems has been developed. The algorithm has been used to solve some optimal control problems with promising results.

92-30792

488

14. SUBJECT TERMS	15. NUMBER OF PAGES
	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	SAR

Final Report for AFOSR 88-0267 October 1992

I. Introduction

The research proposed for this grant centered on the development of algorithms for solving large scale nonlinear constrained optimization problems. This entailed an investigation of the theoretical as well as the computational aspects of these problems. Over the three year period of this grant, several papers were written on issues arising in this study; in particular, on the convergence of rank two updates of matrices used in optimization algorithms and the properties of special merit functions for both equality and inequality optimization problems. These results were outlined in earlier reports to AFOSR. In this report, I will concentrate on the progress toward the major goal; the production of an efficient algorithm for large scale nonlinear programs.

The majority of the work on this grant was done in collaboration with Paul Boggs of the National Institute for Standards and Technology. Tony Kearsley, a graduate student at Rice University and a summer employee at NIST, has been a significant contributor in the programming and testing of the experimental algorithms.

II. An Efficient Algorithm for Large Scale Nonlinear Optimization

The underlying structure of our algorithm is that of the well-known Sequential Quadratic Programming method. In this method the nonlinear program

$$\text{(NLP)} \qquad \begin{aligned} &\text{minimize } f(x) \\ &\quad \text{subject to } \; g(x) \leq 0 \end{aligned}$$

is approximated at each iteration by a (usually positive definite) quadratic program

$$\text{(QP)} \qquad \begin{aligned} &\text{minimize } \nabla f(x)^t \delta + \frac{1}{2} \delta^t H \delta \\ &\quad \text{subject to } \; \nabla g(x)^t \delta + g(x) \leq 0 \end{aligned}$$

where x is the current approximate solution, H is an approximation to the Hessian matrix, and the solution, δ, is the step direction to be taken to the next iterate. (Here we are considering only an inequality constrained problem for notational convenience; the addition of equality constraints requires no significant theoretical changes.) The success of this algorithm in smaller nonlinear programs in well-documented in the research literature of the past decade or so. However to adapt this algorithm to the large scale case involves serious challenges. These include: *i*) whether to use the true Hessian of the Lagrangian as H (which may not be positive definite) or to approximate the Hessian with a positive definite matrix (which generally causes a loss of sparsity); *ii*) how to solve (or approximately solve) QP depending upon the choice of H; *iii*) how to decide on the suitability of a step given by the solution of the QP; and *iv*) how to estimate the multipliers at each step.

The algorithm we have developed utilizes a variation of the now-famous interior-point method to solve QP when H is the true Hessian of the Lagrangian. Specifically, by using a trust region to guard against unbounded or inordinately long steps a variant of the interior-point procedure iterates towards a solution of QP. If it reaches the trust region boundary the process is stopped and the current value of δ is taken as the desired step direction. Then a step length is computed using a merit function we have designed specifically for problems having inequality constraints.

We have been able to show that the step will generally yield a descent direction for this merit function and that the minimum of the merit function is a minimum for NLP. The merit function is then used to update the trust region radius by comparing the predicted and actual merit function reductions. The new multipliers are taken as the multipliers for the QP unless the iterates are far from the solution in which case least squares estimates of the multipliers are used.

The experimental tests that we have run using this approach have been very promising. The theoretical aspects of this method together with these results of are now in the process of being written up in a technical report for submission for publication.

III. Practical Applications of Work and Future Research

Large scale nonlinear programs occur in a variety of applications. For example, they are common in planning and scheduling production in large chemical and petroleum industries, in the solving of discretized optimal control problems in engineering, and in the solution of parameter estimation problems whose underlying models are complex partial differential equations. In our numerical testing, we have solved some optimal control problems. Now that the basic algorithm has been proven to be a promising tool, we are directing some of our research efforts at applying it to specific optimization problems. In particular, we plan to study the interface of solids and liquids in material science (e.g., problems arising in crystal structure at NIST) and the solution of parameter estimation problems for the Stefan problem (from models being investigated at the University of North Carolina).

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